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Comparison between the homogeneous-shear and the sliding-boundary methods to produce shear flow

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Recently, Liem, Brown, and Clarke [Phys. Rev. A **45**, 3706 (1992)] have compared the results obtained from the homogeneous-shear and the sliding-boundary nonequilibrium molecular-dynamics methods to generate shear flow. Here the comparison is carried out by using a kinetic theory description.

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In a recent paper, Liem, Brown, and Clarke [1] have computed the shear properties of a Lennard-Jones fluid from two nonequilibrium molecular-dynamics methods: the "homogeneous-shear" (HS) method and the "sliding-boundary" (SB) method. In the HS method [2], the system is sheared by applying Lees-Edwards periodic boundary conditions. At a macroscopic level, the velocity profile is linear, i.e., $\dot\gamma \equiv \partial u_x/\partial y =$ const, while the density ρ and temperature T are homogeneous. In order to achieve a steady state, an (artificial) thermostat force is introduced. On the other hand, in the SB method, the steady shear flow state is generated by more realistic boundary conditions [1]. As a consequence, the density $\rho(y)$, the temperature $T(y)$, and the shear rate $\dot\gamma(y)$ are nonhomogeneous.

In a shear flow problem, the relevant transport properties are described by the shear viscosity η and the normal stresses $P_{\alpha\alpha}$, $\alpha = x, y, z$. In the hydrodynamic regime [3], these quantities are expected to depend on space and time only through their dependence on the hydrodynamic fields, i.e., $\eta(\rho, T; \dot\gamma)$, $P_{\alpha\alpha}(\rho, T; \dot\gamma)$. The question arises as to whether the above functions are independent of the method followed to produce the shear. The investigation of this point in the cases of the HS and SB methods is the main objective of Ref. [1]. The authors conclude that, for the range of shear rates considered, the pressure tensor components are largely insensitive to the simulation method. As Liem, Brown, and Clarke point out, the above comparison is constrained to shear rates for which normal pressure differences (i.e., viscometric effects) are not significant. Larger shear rates in the SB method are difficult to obtain due to the disruption caused to the boundaries by the viscous heat generated in the fluid, that cannot be dissipated by thermal conduction [1].

The aim of this Brief Report is to shed light on the above problem by using a dilute fluid as a prototype system. We shall adopt the well-known BGK kinetic model [4], whose exact solutions for the HS problem [5–7] and the SB [8, 9] problem have been obtained in the past few years. In both cases, the transport properties can be cast into the form

$$\eta(\rho, T; \dot\gamma) = \eta_0(\rho, T)\Psi(a) , \tag{1}$$

$$P_{\alpha\alpha}(\rho, T; \dot\gamma) = p_0(\rho, T)\Phi_\alpha(a) , \tag{2}$$

where $\eta_0(\rho, T) \equiv \eta(\rho, T; 0)$ is the Navier-Stokes shear viscosity coefficient and $p_0(\rho, T) \equiv \frac{1}{3}$ Tr $\mathsf{P}(\rho, T; 0)$. Non-Newtonian effects are contained in $\Psi(a)$ and $\Phi_\alpha(a)$, where $a(\rho, T; \dot\gamma) \equiv \dot\gamma/\zeta(\rho, T)$, $\zeta(\rho, T) \equiv p_0(\rho, T)/\eta_0(\rho, T)$ being an effective collision frequency. The reduced shear rate a represents a uniformity parameter, namely, the ratio between a mean free path and a characteristic hydrodynamic length. In the HS case, the functions appearing in Eqs. (1) and (2) are given by [7]

$$\Psi^{\rm HS}(a) = \frac{1}{(1+\lambda)^2} , \tag{3}$$

$$\Phi_x^{\rm HS}(a) = \frac{1+3\lambda}{1+\lambda} , \tag{4}$$

$$\Phi_y^{\rm HS}(a) = \Phi_z^{\rm HS}(a) = \frac{1}{1+\lambda} , \tag{5}$$

where $\lambda(a) = \frac{4}{3}\sinh^2[\frac{1}{6}\cosh^{-1}(1+9a^2)]$. It is worth mentioning that Eqs. (3)–(5) are also exactly verified in the context of the Boltzmann equation for Maxwell molecules [3].

In the SB case, the exact solution to the BGK equation yields [8, 9]

$$\Psi^{\rm SB}(a) = F_0(\beta) , \tag{6}$$

$$\Phi_x^{\rm SB}(a) = 1 + 4\beta\,[F_1(\beta) + F_2(\beta)] , \tag{7}$$

$$\Phi_y^{\rm SB}(a) = 1 - 2\beta\,[F_1(\beta) + 2F_2(\beta)] , \tag{8}$$

$$\Phi_z^{\rm SB}(a) = 1 - 2\beta F_1(\beta) , \tag{9}$$

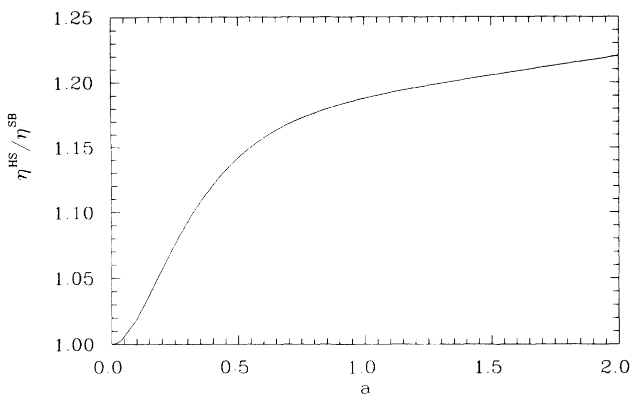

FIG. 1. Shear rate dependence of the ratio of shear viscosities $\eta^{\rm HS}/\eta^{\rm SB}$.

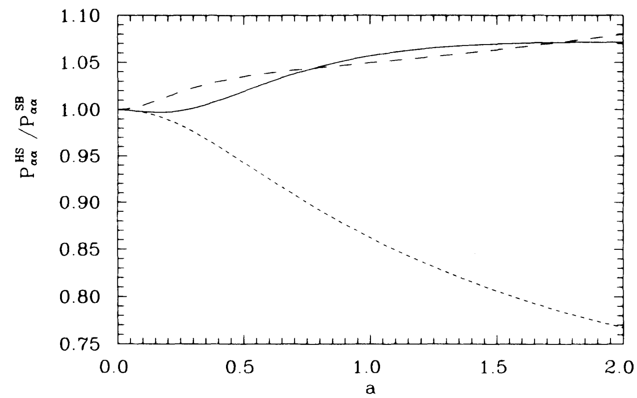

FIG. 2. Shear rate dependence of the ratio of normal stresses: $P_{xx}^{\rm HS}/P_{xx}^{\rm SB}$ (—), $P_{yy}^{\rm HS}/P_{yy}^{\rm SB}$ (– – –), and $P_{zz}^{\rm HS}/P_{zz}^{\rm SB}$ (- - -).

where $\beta(a)$ is defined through the implicit equation

$$a^2 = \beta \left[3 + 2\frac{F_2(\beta)}{F_1(\beta)}\right] \,. \tag{10}$$

In Eqs. (6)–(10), $F_r(\beta) \equiv (\frac{d}{d\beta}\beta)^r F_0(\beta)$, with

$$F_0(\beta) = \frac{2}{\beta}\int_0^\infty dt\, t\, e^{-t^2/2} K_0(2t^{1/2}/\beta^{1/4}) \,, \tag{11}$$

K_0 being the zeroth-order modified Bessel function.

It is evident from Eqs. (3)–(5) and Eqs. (6)–(10) that both methods lead to different results beyond the Navier-Stokes limit. For instance, the super-Burnett contribution to the shear viscosity is 2.7 times greater in the SB case than in the HS case. Further, at small shear rates, the first viscometric function $[(\Phi_y - \Phi_x)/a^2]$ and the second viscometric function $[(\Phi_z - \Phi_y)/a^2]$ take the values $-\frac{14}{5}$ and $\frac{4}{5}$, respectively, in the SB case, whereas they take the values -2 and 0 in the HS case. For large shear rates, the pressure tensor components exhibit different asymptotic behaviors in both methods. In particular, $\eta^{\rm HS} \sim a^{-4/3}$, while $\eta^{\rm SB} \sim a^{-2}\log a$. In order to perform a more detailed comparison, we plot the ratios $\eta^{\rm HS}/\eta^{\rm SB}$ and $P_{\alpha\alpha}^{\rm HS}/P_{\alpha\alpha}^{\rm SB}$ as functions of the reduced shear rate a. Figure 1 shows that the shear thinning effect is more noticeable in the SB case than in the HS case. In Fig. 2, we observe that the differences between both methods are less important for the xx and yy pressure components than for the zz component and the shear viscosity. In particular, the ratio for the xx component is always close to 1. This is basically due to the fact that, as the shear rate increases, the dominant contribution to the trace of the pressure tensor is that of the xx component.

The origin of the discrepancies between the results obtained from the HS and the SB methods lies in the fact that they lead to quite different macroscopic states [10]. Thus, while the heat flux is absent in the first case, there exists heat transport across the system in the second case, even in the Navier-Stokes regime. Regarding the shear viscosity, it must be emphasized that $\eta^{\rm SB}$ contains contributions associated to temperature gradients and to second- and higher-order derivatives of the flow velocity. On the other hand, all those contributions disappear in $\eta^{\rm HS}$. It must be also pointed out that the transport properties in the HS problem with and without thermostat forces are different [6,11]. However, these differences are less important than the ones reported here.

Finally, it must be noticed that conclusions supported by a kinetic theory description should not be extended to dense fluids without caution. Nevertheless, one expects the essential qualitative features of the comparison between the HS and the SB methods to be rather insensitive to the range of densities considered. As Liem, Brown, and Clarke [1] have pointed out, the values of shear rates considered in Ref. [1] are not large enough to observe discrepancies between the HS and the SB methods. By extrapolating our definition of effective collision frequency $\zeta = p_0/\eta_0$ to dense fluids [5], we can estimate that the range of shear rates in Ref. [1] correspond to $a \approx 0.03$. For this value, our kinetic theory description predicts that $\eta^{\rm HS}/\eta^{\rm SB} = 1.002$ and non-Newtonian effects are negligible. We think that careful nonequilibrium computer simulations as those reported in Ref. [1] should be carried out for much larger shear rates in order to observe appreciable differences between several methods to produce shear flow.

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